

# Electron scattering due to dislocation wall strain field in GaN layers

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The effect of edge-type dislocation wall strain field on the Hall mobility in  $n$ -type epitaxial GaN was theoretically investigated through the deformation potential within the relaxation time approximation. It was found that this channel of scattering can play a considerable role in the low-temperature transport at the certain set of the model parameters. The low temperature experimental data were fitted by including this mechanism of scattering along with ionized impurity and charge dislocation ones.

## I. INTRODUCTION

As is known GaN films are under extensive examination for many years because of their promising application for the construction of short-wavelength light emitting devices<sup>1,2</sup>. However, the performance of these devices is limited by defects, both native and impurity types. Native defects, in particular, are threading dislocations with high densities ( $10^8 - 10^{11} \text{ cm}^{-2}$ ) which are result from the large lattice mismatch between epilayer and substrate<sup>3,4,5</sup>. Dislocations, being charged objects, act as scattering centers (core effect) for carriers affecting the transverse mobility in films<sup>6</sup>. In most studies in the context of the GaN layers this Coulomb scattering has been considered<sup>7,8,9,10</sup>. At the same time, in addition to the core scattering, dislocations can give contribution to the resistivity through deformation and piezoelectric potentials<sup>6,11</sup>. In GaN layers these potentials associate with the strain field of dislocation arrays which form low-angle grain boundaries or separate dislocations in the specific cases<sup>7</sup>. However, the carrier scattering due to piezoelectric potential has been found as negligibly small within the bulk of GaN<sup>12</sup>.

## II. MODEL

In this paper we theoretically investigate the contribution to the Hall mobility in GaN layers from a wall of dislocations of edge type. The scattering of electrons by dislocation wall (DW) is treated in the framework of the deformation potential approach. In this case, the perturbation energy of electron can be written in the standard form<sup>13,14</sup>

$$\delta U(\mathbf{r}) = G\Delta(\mathbf{r}), \quad (1)$$

where  $\Delta(\mathbf{r})$  is the dilatation of lattice around a finite dislocation array,  $G$  is the deformation-potential constant.

Let the threading dislocation segments with coordinates  $(0, h)$  along the  $(0, 0, 1)$  axis (perpendicular to the interface/layer plane) form a dislocation wall of finite length  $2L$ . The dilatation at the point  $\mathbf{r} \geq 2L$  around such defect, then, can be found based on the so-called disclination model of grain boundaries and dislocations for isotropic medium<sup>15,16</sup>. It takes the form<sup>17</sup>

$$\Delta(\mathbf{r}) = \frac{(1-2\sigma)}{(1-\sigma)} \frac{b}{4\pi p} \left( \ln \frac{\sqrt{\rho_+^2 + z^2} - z}{\sqrt{\rho_+^2 + (h-z)^2} + (h-z)} - \right.$$

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$$\ln \frac{\sqrt{\rho_-^2 + z^2} - z}{\sqrt{\rho_-^2 + (h-z)^2} + (h-z)} \Big), \quad (2)$$

where  $\rho_\pm^2 = (x \pm L)^2 + y^2$ ,  $b$  is the Burgers' vector of dislocation in the wall,  $p$  is the distance between dislocations in the wall,  $\sigma$  is the Poisson constant. It is interesting to note that Eq.(2) is also the exact formula for the dilatation around the high-angle grain boundary as well as the disclination dipole.

The square of the matrix element of electron scattering in momentum states  $\mathbf{k}$  to states  $\mathbf{k}'$  with the perturbation energy given by Eq.(2) deduced in<sup>17</sup> as

$$|\langle \mathbf{k} | U(r) | \mathbf{k}' \rangle|^2 = \frac{32\pi^2 A^2}{(q_z^2 + q_\perp^2)^2 V^2} \frac{\sin^2(q_z h/2)}{q_z^2} (1 - J_0(2q_\perp L)), \quad (3)$$

where  $A = \frac{Gb(1-2\sigma)}{4\pi p(1-\sigma)}$ . As one can see from Eq.(2) and Eq.(3), the scattering due to perturbation  $\delta U(\mathbf{r})$  is three dimensional, therefore  $(\mathbf{k} - \mathbf{k}')_z = q_z = \sqrt{q^2 - q_\perp^2} \neq 0$  in contrast to the case of an infinitely long dislocation line along the (0,0,1)-axis. Omitting the details of further calculations, we can come to the following equation for the relaxation time due to the strain field of DW

$$\tau_{wall}^{-1}(k) = \frac{32A^2 L^2 n_{def} \pi m^*}{\hbar^3 k_\perp^2} \left( \text{Si}(hk_\perp) + \frac{\cos(hk_\perp)}{hk_\perp} - \frac{1}{hk_\perp} \right) \left( J_0^2(2Lk_\perp) + J_1^2(2Lk_\perp) - \frac{1}{2Lk_\perp} J_0(2Lk_\perp) J_1(2Lk_\perp) \right), \quad (4)$$

where  $n_{def}$  is the arial density of DW which is inversely proportional to the square of the mean distance between grain boundaries,  $m^*$  is the effective mass of carrier,  $J_n(t)$  are the Bessel functions,  $\text{Si}(x)$  is the sine integral function,  $k_\perp = (k_x, k_y)$  is the normal to the disclination line component of the wave vector,  $\hbar$  is the reduced Planck's constant. When a film is thick ( $k_\perp h \gg 1$ , bulk regime) Eq.(4) can be simplified to

$$\tau_{wall}^{-1}(k) = \frac{16A^2 L^2 n_{def} \pi^2 m^*}{\hbar^3 k_\perp^2} \left( J_0^2(2Lk_\perp) + J_1^2(2Lk_\perp) - \frac{1}{2Lk_\perp} J_0(2Lk_\perp) J_1(2Lk_\perp) \right), \quad (5)$$

The relaxation time due to Coulomb scattering at charged dislocation lines can be written in the well-known form as<sup>18</sup>

$$\tau_{dis}(k) = \frac{\hbar^3 \epsilon^2 c^2}{N_{dis} e^4 f^2 m^*} \frac{(1 + 4\lambda_d^2 k_\perp^2)^{3/2}}{\lambda_d}, \quad (6)$$

where  $N_{dis}$  is the dislocation density in the wall,  $c$  is the distance between acceptor centers along the dislocation line,  $f$  is the occupation rate of the acceptor centers along the dislocation,  $\epsilon$  is the dielectric constant,  $e$  is the electronic charge,  $\lambda_d = \sqrt{\frac{\epsilon k_B T}{e^2 n}}$  is the Debye screening length with electron concentration  $n = N_D^+ - N_A^- - f(N_{dis}/c)$ , and  $k_B$  is the Boltzmann's constant. To determine the filling factor  $f$ , the procedure from<sup>10</sup> has been used.

Assuming the validity of the non-degenerate statistics, we can evaluate the DW contribution  $\mu_{wall}$  to the total mobility using the well-known formula

$$\mu(k) = \frac{e\hbar^2}{m^{*2} k_B T} \frac{\int \tau(k) k_i^2 f_0 d^3 k}{\int f_0 d^3 k} = \frac{e\langle \tau \rangle}{m^*}, \quad (7)$$

where  $k_i = k_{x(y)}$  is the planar component of the wave vector, and  $f_0$  is the Boltzmann distribution function.

### III. NUMERICAL RESULTS

We first analyzed the drift mobility contribution due to grain boundary strain field together with other important mechanisms of scattering at low temperatures (ionized impurities, charged dislocation lines). The component of the scattering due to ionized impurities has been taken in the form of the Brooks-Herring-like formula obtained on the basis of the partial-wave phase-shift method<sup>19</sup>. This approach yields the correct results for low  $T$  and high  $n$  where the Born approximation can be false. It takes the form

$$\frac{1}{\tau_{ii}(k)} = N_I v \sigma^B(k) H_0, \quad (8)$$

where  $N_I$  is the ionized impurity concentration,  $v$  is the electron velocity,  $\sigma^B(k)$  is the Born cross section, and  $H_0$  is the factor of correction obtained from the phase-shift calculations<sup>19</sup>. We found that the Coulomb dislocation scattering is major at free carriers concentration  $n < 10^{17} \text{cm}^{-3}$  when  $N_{dis} \approx 10^8 \text{cm}^{-2}$  ( $T < 100\text{K}$ ), and above this  $n$  the impurity scattering dominates. In our calculations dislocation core scattering always dominates above  $N_{dis} \approx 10^8 \text{cm}^{-2}$ . The numerically calculated  $\mu_{wall}$  on the basis of the Eqs.(4),(6) is shown in Fig.1 as a function of temperature for some selected model parameters together with other contributions. The deformation-potential constant  $G$  has been taken equal to 4 eV, that corresponds to the typical values for semiconductors. From our analysis we found that  $\mu_{wall} \sim T^{3/2}$  (unlike the case of the separate dislocations where  $\mu \sim T$ ), and this contribution can be maximal for some chosen set of the parameters when the concentration of the DW is sufficiently high ( $n_{def} \simeq 10^{10} \text{cm}^{-2}$ ) (see Fig.1).

The low temperature part of the experimental data from<sup>21</sup> for two GaN samples with  $N_{dis} = 4 \times 10^8 \text{cm}^{-2}$  and  $2 \times 10^{10} \text{cm}^{-2}$  on the sapphire substrate has been fitted based on the formula for the Hall mobility  $\mu_H = e\langle\tau^2\rangle/m^*\langle\tau\rangle$ . Here the total relaxation time is given by

$$\langle\tau\rangle = \left\langle \frac{1}{\tau_{wall}^{-1} + \tau_{dis}^{-1} + \tau_{ii}^{-1}} \right\rangle. \quad (9)$$

The results are presented in Fig.2. As shown, there is agreement with the experimental data when  $30\text{K} < T < 100\text{K}$  for both samples. We found that the result of the fit essentially depends on the distance between dislocations in the wall  $p$ , as compared to other parameters, and, hence on the angle of misorientation between grains ( $\theta = \arcsin(b/2p)$ ).

Our preliminary results show that this effect of the angle variation on the Hall mobility can be noticeable even for a narrow interval of  $\theta$  between  $1^\circ$  and  $5^\circ$ . The second very sensitive parameter in our calculations is the position of the dislocation acceptor level energy referred to the conduction band edge energy.

As noted above, Eq.(2) describes both the dilatation around the low-angle grain boundary and disclination dipole. The concept of disclination dipole has been applied to obtain the deformations around high-angle grain boundaries and linear defects of the rotational type<sup>22</sup>. In this connection, the observed in hexagonal GaN layers deformations associated with the 5/7 and 4/8 rings and high-angle grain boundaries (see, for example, Refs.<sup>23,24</sup>) can be considered in the framework of the disclination dipole model. The second point which should be noted concerns the interfacial misfit dislocations<sup>25</sup>. Misfit dislocation scattering along with considered in this paper can be given in the framework of the multi-layer model proposed in<sup>26</sup>.

### IV. CONCLUSIONS

In this article we have theoretically investigated the possible role of the strain field associated with the dislocation

wall on the mobility in hexagonal GaN layers. It has been found that this contribution to the total transverse mobility can be noticeable at low temperatures for given above densities of such defects and deformation constant typical for semiconductors. Our calculations show the core scattering due to charged dislocation lines is dominant mechanism when  $N_{dis} > 10^9 \text{cm}^{-2}$ . This supports findings in previous publications devoted to this material. At lower dislocation densities the ionized impurity scattering and strain field scattering can dominate.

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## Figure Captions

Fig.1. Calculated contributions to the total drift mobility as a function of temperature for the model parameters:  $N_{dis} = 10^8 \text{cm}^{-2}$ ,  $n_{def} = 1.5 \times 10^{10} \text{ cm}^{-2}$ ,  $f = 0.8$ ,  $n = 4 \times 10^{16} \text{ cm}^{-2}$ ,  $p = 10^{-2} \mu\text{m}$ ,  $h = 1.2 \mu\text{m}$ . The rest of the parameter set has been taken from Ref.<sup>20</sup>

Fig.2. Hall mobility vs temperature for two samples with  $N_{dis} = 4 \times 10^8 \text{cm}^{-2}$  (squares),  $N_{dis} = 2 \times 10^{10} \text{cm}^{-2}$  (circles) from Ref. Solids lines are theoretical curves. The set of the model parameters: (for squares)  $G = 9 \text{ eV}$ ,  $f = 0.92$ ,  $p = 9 \times 10^{-3} \mu\text{m}$ ,  $n_{def} = 2.7 \times 10^{10} \text{ cm}^{-2}$ , (for circles)  $G = 7 \text{ eV}$ ,  $f = 0.98$ ,  $p = 6 \times 10^{-3} \mu\text{m}$ ,  $n_{def} = 1.5 \times 10^{10} \text{ cm}^{-2}$ .



